DOI: 10.15669/pnst.4.99

Progress in Nuclear Science and Technology
Volume 4 (2014) pp. 99-103

ARTICLE

Validation studies of computational scheme for high-fidelity fluence estimations of the Swiss BWRs

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The paper presents recent activities conducted at the Paul Scherrer Institut (PSI) in relation to the development and validation of an integral calculation methodology based on CASMO-4/SIMULATE-3/MCNPX for accurate estimations of the fast neutron fluence (FNF) accumulated on reactor pressure vessels and internals of the operating Swiss BWRs. With this computational scheme, the default neutron source is set up at the pin-by-pin level with realistic spectrum specifications based on the actual reactor cycle-specific data from validated reference CASMO-4/SIMULATE-3 core analysis models. On this basis, MCNPX models are then applied for optimized calculations of the fast neutron flux at the RPV or at any other location of interest including e.g. at surveillance dosimeters. In that framework, the validation studies conducted so far have included one dosimeter set irradiated in a BWR/6 reactor during two relatively recent operating cycles. Although this first analysis revealed a satisfactory performance when comparing the calculation results to measured data, it was considered necessary to proceed with further sensitivity/optimization studies combined with an enlarged validation basis (i.e. using additional dosimeter sets) in order to strengthen the overall confidence in the scheme both at the qualitative and quantitative level. A summary of the recent progress achieved in these directions is presented in this paper. To start, recalling that BWRs are characterized by very complex and heterogeneous fuel assembly and core designs (e.g. pins with different enrichments and burnable absorber loading, partial length rods, fuel assemblies of different types in the core), the impact of such heterogeneities on FNF estimations is under investigation in order to determine the level of modeling details required for accurate computational schemes to be used for long-term evaluations of modern BWR core designs. Next, additional validation studies based on experimental dosimeter data obtained from the same BWR/6 reactor are presented. These enlarged validation studies involve the analysis of four dosimeter sets, each irradiated during one cycle (including the 3 first reactor operation cycles), and subsequently analyzed at the PSI Hot Lab shortly after the dosimeters extraction. All these additional validation studies are conducted using both the JEFF-3.1.1 and the ENDF/B-VII.0 continuous-energy neutron data libraries in order to assess the sensitivity of the PSI BWR computational scheme also upon the employed nuclear data.

Keywords: fast neutron fluence; CASMO-4/SIMULATE-3/MCNPX; BWR; dosimetry; validation studies

1. Introduction

At PSI, a computational scheme for FNF estimations based on CASMO-4/SIMULATE-3/MCNPX-2.4.0 is under development. The ultimate goal is to provide, in compliance with the recognized existing practices [1,2], the ability for accurate FNF assessments of the Swiss LWRs. The principles of the PSI scheme as well as the accuracy achieved for PWRs can be found in [3]. Recently, the scheme was updated for BWR applications and to launch the verification/validation (V&V) phase, a first validation case was conducted for a dosimeter data set irradiated in two recent cycles of a Swiss BWR/6 reactor [4]. Although this first case has shown a satisfactory performance, it is now necessary to enlarge the V&V basis in order to verify the applicability of the scheme for different types of core/fuel designs or reactor operating strategies and through this, identify and refine relevant methodological components. This is the objective of the present paper which summarizes the results of four new validation cases based on experimental data obtained from dosimetry irradiation programs carried out in four different cycles of the same BWR/6 plant. All of these four cycles (the first three being the initial reactor cycles) were operated substantially earlier than the one investigated in [4],

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providing thereby the opportunity to study the impact of core design evolution and changes in reactor operation on the scheme's accuracy. For the latter three cycles, two types of dosimeter detectors, namely ^{54}Fe and ^{93}Nb, were used while for the first cycle, only a ^{54}Fe dosimeter was employed. In all cases, the dosimeters were irradiated in the vicinity of the reactor pressure vessel (RPV) and subsequently analyzed at the PSI Hot Lab, providing thereby an experimental-based set of results consisting of 4 FNF evaluations and 7 corresponding detector activities. This paper presents the validation of the PSI FNF scheme for these four dosimeter programs.

2. BWR scheme and MCNPX model

For any operating cycle, the principle of the PSI BWR FNF calculation scheme is to transfer to an MCNPX [5] model the spatial/temporal neutron source distribution as well as the in-channel 1-D axial node-averaged thermal-hydraulic (T-H) conditions [3,4] from a validated CASMO/SIMULATE (C/S) model of the actual cycle [6]. For every FA in the core, the neutron source is transferred at the rod-by-rod level in the horizontal cross-section and with a FA-average axial distribution shape. The neutron source spectrum is modeled by taking into account actual fuel compositions. More details on this can be found in [3,4]. For the validation analyses presented here, the influence of the power re-distributions during cycle operation was not found to be significant for the considered dosimeter monitors [4]. Therefore, the changes in power distribution were ignored and the option to transfer cycle-averaged source distributions was applied. Moreover, an additional simplification made here is that a uniform core-averaged 1-D axial coolant density distribution is applied for all channels. Concerning the MCNPX geometrical representation, the model includes all core/bypass/downcomer zones. However, for the sake of calculation efficiency, only a truncated core region is employed for the validation studies. This truncated core model is illustrated in **Figure 1** and was in fact already adopted for the previous validation analysis [4] (although it was verified to also be appropriate for the cycles investigated here).

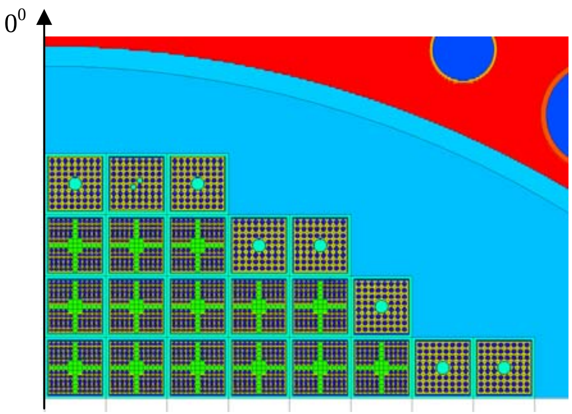

Figure 1. MCNPX Core Model Representation (an example).

One main reason to use such a truncated model is that for all four cycles, the dosimeters were placed in the vicinity of the RPV, axially at the core centerline and radially, close to the 0º symmetry axis, namely at 6º for first three cycles and at 3º for the fourth cycle. Apparently, these azimuth/axial coordinates of the dosimeters placement correspond well to the locations where the maximum neutron flux is likely to take place (e.g. at the RPV and at the core shroud). This is illustrated in **Figure 2** where a qualitative view of the typical fast neutron flux shape predicted by MCNPX on the core shroud (CS) inner surface is shown.

With regards to the flux values at the dosimeter locations, only the few closest FAs were previously found to play a significant role when estimating the so-called FA "importance factors" (*IF*) [4]. To confirm, this, corresponding *IF* calculations were performed here. The results for the first cycle are shown in the upper part of **Figure 3** and are very similar to those obtained in [4]. Moreover, on the lower part of Figure 3, the absolute differences in *IF* between the first cycle and one of the recent cycles used in previous study [4] are presented and show that the *IF* re-distributions during reactor operation or between cycles may be considered as moderate enough to justify the core model geometrical truncation.

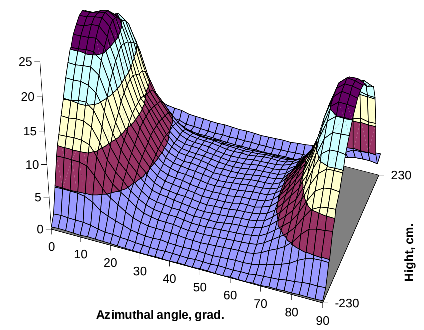

Figure 2. Representative fast neutron flux on CS surface (Rel. units).

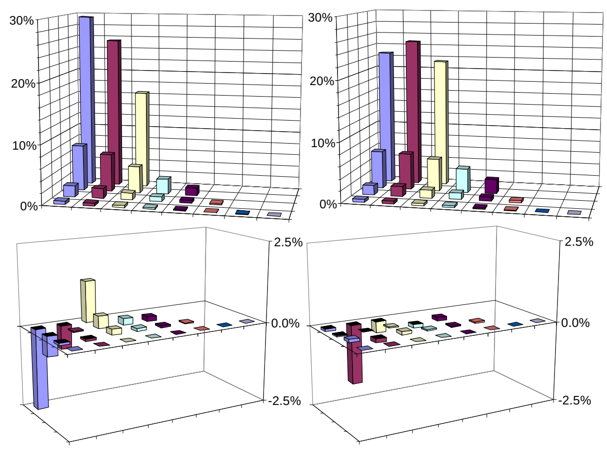

Figure 3. *IF* values for FNF at 3° (left) and 6° (right) for the first cycle (top) and *IF* differences between one of the recent cycles and cycle 1 (bottom).

3. Sensitivity and optimization studies

Regarding the continuous evolution towards increasingly more complex and heterogeneous BWR cores, it is considered important to assess the level of details required in the MCNPX model to account for various FA designs. These will indeed differ in terms of a) structural/mechanical design such as heterogeneous intra-assembly rod-by-rod layouts/dimensions, water rod configurations, partial length rods and b) nuclear design e.g. axial/radial fuel and burnable absorber zoning with varying fuel density/enrichments and/or Gd content. For the structural/mechanical design, the geometrical heterogeneities are accounted for by modeling in a representative manner, each FA according to its design type and based on the C/S core models (Figure 1). Effects of the partial length rods (PLR) modeling was not assessed in this study as none of the considered cycles here included PLR FAs.

For the nuclear design parameters such as fuel density and fuel enrichment, sensitivity studies were carried out for the cycles analyzed in [4]. The results, summarized in **Table 1** below, show that variations in these parameters have a little impact for fast neutron flux analysis (only in the context of neutron transport modeling with a pre-defined neutron source). For completeness, similar sensitivity studies were done for one of the cycles analyzed here and confirmed the same trends. Concerning the sensitivity of the fast neutron flux to the presence of burnable absorbers, it was estimated that neglecting the absorber presence (and associated variation of the fuel density in the rods with absorbers) also should not cause any significant bias in FNF results comparing to the present calculation precision. At the current stage of the validation studies, the nuclear design heterogeneities are neglected and therefore, uniform ‘representative’ values are at this stage considered as sufficient and thus employed. However, it is planned as one of the next steps to upgrade the C/S – MCNPX linking tool such as to allow for an automatic transfer of this type of nuclear design data, as well as more detailed coolant density specifications, in order to reduce unnecessary computational biases.

Table 1. Sensitivity to Nuclear Design Parameters.

Change in MCNPX model	**Response of FNF***
Fuel density reduction by 5%	~ +3%
^{238}U cross-sections used for all fuel nuclides and fission products	~ 0% (not detected)*
^{235}U cross-sections used for all fuel nuclides and fission products	~ +2%

*) MCNPX relative error (R) was ~1%

4. Validation studies and results

With the approach described in Sections 2 and 3, the neutron fluxes and the reaction rates corresponding to the utilized dosimeter monitors, ^{54}Fe(n,p) and ^{93}Nb(n.n’), were thus calculated and consequently evaluated using the procedure described in [4]. Calculations were performed with two neutron data libraries: JEFF-3.1.1 [7] and ENDF/B-7.0 [8] but in both cases, the same ^{93m}Nb production cross-section from the ENDF/B-VI MOD 3 library was used. In all cases, the relative errors of the MCNPX calculation results were within ~1.5%, which can be considered as acceptable when taking into account other sources of uncertainties [2, 4].

The C/E results obtained with the above-described calculation approach are collected in the **Table 2**.

Table 2. Activities C/E* Results.

Lib.	Det.	**1**	**2**	**3**	**4**	Av.
JEFF-3.1.1	Fe-54	1.01	090	0.97	0.91	**0.95**
	Nb-93	-	1.10	1.15	1.07	1.11
	Av.	1.01	1.00	1.06	0.99	1.02
ENDF/B-7.0	Fe-54	1.15	1.03	1.11	1.05	**1.09**
	Nb-93	-	1.17	1.22	1.15	1.18
	Av.	1.15	1.10	1.16	1.10	1.13

*) Actually, the activities were measured for several samples, but here only averaged measurements are considered noting that typical measurement uncertainties were mentioned to be within ~5% and that a substantially higher variation between the individual dosimeter measurements was specified.

The magnitude of the C/E agreements above, i.e. for four dosimeter sets from four different cycles, is very consistent with the previous results obtained for the more recent cycle [4]. For a given dosimeter type, a certain variation is seen between the four cases. This may indicate that cycle-specific features to some extent affect the achieved accuracy. The cycle variation of the C/Es seen here remains however moderate and this provides thus additional confidence that the developed methodology adequately accounts for cycle-specific features and allows thereby to reach a similar accuracy for any cycle. The level of accuracy will however differ depending on the dosimeter type. Indeed, the overall agreement can be seen to better for the ^{54}Fe dosimeter than for the ^{93}Nb one.

Now when comparing the results as function of library, the above results also confirm the previously observed trends in C/E behavior: a) the main discrepancies between libraries are seen for the Fe dosimeter activity and are due to the library differences in terms of the ^{54}Fe(n,p) reaction cross-section [4]; b) the higher C/Es for ^{93}Nb despite using the same cross-sections indicate that in general, ENDF/B-7.0 library produces higher fluxes at these dosimeters locations (see also [4]).

Finally, it must be noted that apparently, the original purpose of the dosimetry programs was first of all to allow for an evaluation of FNF values based on the measured activities. Nowadays, the FNF at arbitrary locations can be calculated with more advanced computational methodologies e.g. such as the PSI scheme under development here or similar approaches

[2]. Therefore, it is valuable to verify how the computed FNF results obtained here agree with the values previously derived based on the experimental evaluations. This is shown in **Table 3** where the FNF C/Es, i.e. calculated versus experimentally-based FNF evaluations, are presented. As one can see, the FNF results obtained in the given calculations and in the previous experimental-base evaluations agree very well with a tendency for slightly lower fluences when using JEFF-3.1.1 and moderately higher ones with the ENDF/B-7.0 library.

Table 3. FNF C*/E Results.

Case	**1**	**2**	**3**	**4**	**Av**
JEFF-3.1.1	0.95	0.96	1.04	0.94	0.97
ENDF/B-7.0	1.00	1.02	1.10	1.02	1.04

*) MCNPX relative error (R) was ~1%

The above agreement in average FNF between calculations and experimental evaluations is in fact even better than for the activities and this applies to both types of detectors. Without presenting details, it can just be mentioned that one reason for such behavior is that the experimental-based evaluations were done using one-group effective neutron micro cross-sections based on the ENDF/B-V library and these are not the same as when calculated with more modern libraries such as those employed here in the PSI scheme. This introduces compensating effects such that the final experimental-based FNF evaluations happen to agree very well with the values calculated with the PSI scheme. Thus the present study may be considered as an additional verification of previous experimentally-based assessments of the FNF for the given BWR.

5. Conclusion

The development of a CASMO/SIMULATE/MCNPX methodology for high-fidelity FNF assessments of the Swiss BWRs is on-going at PSI. Currently, validation studies of the scheme for a BWR/6 plant are being performed based on available experimental-based data from past dosimetry programs conducted in the reactor and evaluated at the PSI Hot Lab. This paper presents four new validation cases based on dosimeter sets obtained from four early reactor cycles, increasing thereby, the total number of dosimetry sets evaluated so far to five including 9 individual dosimeter detectors. For all cases, calculations were performed with two distinct modern libraries and the results were found to show quite reasonable agreement against experimentally-evaluated values (within ~±20%), noting that the FNF values derived in the original evaluations at the PSI Hot Lab for the two considered detector types and based on measured activities typically, also varied within ~20%. Furthermore, as it was previously observed, the ENDF/B-7.0 library produces in general higher FNF values compared to the JEFF-3.1.1 library. And regarding the obtained C/E values for the specific activities of the considered dosimeters, it is found that the JEFF-3.1.1 library gives slightly better results. This is mostly due to differences in the ^{54}Fe cross-section, noting that for the ^{93}Nb dosimeter, the same cross-sections were indeed used for the calculations with the two libraries.

The next planned stages of the validation studies will include analysis of dosimeters which were irradiated during a larger number of reactor cycles, underlining that those considered so far, i.e. analyzed here as well as previously [4], corresponded all to one or at most, two cycles irradiation programs. The objective will be to provide enhanced reliability in the methodology from the point of view of FNF assessments for the entire reactor lifetime. Also, this will allow to further asses scheme/modeling refinements concerning e.g. more detailed specifications of the coolant density distributions within the FAs and within the intra/inter assembly bypass zones, more accurate specification of the fuel composition distributions within the FAs and within the core, or more precise account of axial geometry discontinuities such as partial length rods.

Acknowledgements

This work was partly supported by swiss*nuclear*, the nuclear energy section of the Swiss electricity companies. The authors would also like to express their gratitude to Gregory Perret (PSI) for his support for the MCNPX-2.4.0 code and valuable comments.

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